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An external evaluation of the Data Management Program for the operations of the Installation Restoration program is presented. Specific recommendations are made for the improvement of the Data Management Program. These recommendations cover management of the data log books, extra data fields to input error estimates, data , and free-form comments, system input stability, and required data sampling plans. In addition, a review of contaminant models is presented. Finally, a weakness in the quality control is presented, and a management information system is discussed.

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EVALUATION OF DATA MANAGEMENT FOR INSTALLATION RESTORATION

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PREFACE

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SUMMARY

An external evaluation of the Data Management Program for the operations of the PM-IR is presented. In general, it was found that the operation of the data base are in keeping with the needs of the IR program.

Specific recommendations are made for the improvement of the Data Management Program. These recommendations cover management of the data log books, extra data fields to input error estimates, data, and free-form comments, system input stability, and required data sampling plans. In addition, a review of contaminant models is presented.

Finally, a weakness in the quality control is presented, and a management information system is discussed.

EVALUATION OF DATA MANAGEMENT FOR INSTALLATION RESTORATION

by

T. J. Thomas and G. Kovacs

INTRODUCTION

The Program Manager for Installation Restoration decided that, as a part of his overall data collection program at various installations throughout the country, all data collected should be sent to a common site for storage, retrieval, and processing. Accordingly, through the efforts of his office, a Data Manager was hired, hardware and software was obtained, coordination with remote sites was begun, and central site processing is now an evolving reality.

However, there existed the possibility that the data base activities might evolve away from PM-IR needs, or, that PM-IR needs could not be met. This possibility was underscored by the observation that neither the Data Manager or remote sites could fully justify collected data on present needs. Rather, justification was presented on the grounds that the data might be needed for future analyses.

Accordingly, this study was undertaken to review the data management program from the outside and provide guidance as to IR policy, data needs, soft and hardward needs, and any other information which could be used to aid the data management activities.

The study recommendations are not binding upon the PM-IR, but rather should serve as a basis for possible further evolution of the data management program.

OBJECTIVE

The objective of this study is to provide guidance to the PM-IR on the developing data management program.

APPROACH TO THE PROBLEM

The overall objective was subdivided into several study areas, as follows:

(1) Policy definition

(2) Data requirements

(3) System modeling

(4) System analysis

(5) Resource requirements.

The results for each study area are presented in the following chapters.

POLICY DEFINITION

This task was directed to the evaluation of PM-CDIR policy and objectives guiding the development and use of the IR data management system. The format of this section of the report is a presentation of the PM-IR policies, and discussion and a list of issues to which PM-IR attention should be directed.

PM-IR Policies and Objectives Guiding the Development of IR Data Management System

A. IR Data Management System

(1) System is to provide a common data base applicable to each installation being restored or under investigation; its primary function is to provide data support for designing an effective Restoration System Plan for each installation to be restored.

(2) System is to be centralized computer data bank consisting of data pertaining to four functional areas: (a) sampling and analysis, (b) standards, (c) decontamination technologies, (d) costs of control/abatement options (see C.3).

(3) Data Management, in conjunction with a Decision Model, is to support the means for (a) assessing current and future pollutant levels, (b) determining biological effects, (c) establishing allowable limits/levels of pollutants (see B.1-B.3) and (d) preparation of the Restoration System Plan.

(4) Computerized data management and automated data processing techniques are to be utilized to facilitate data handling, and to minimize both lag time between data generation and file update and errors of transcription during input.

(5) The IR Data Management System is to meet the requirements of all users within the IR community (see E).

(6) Some desired system capabilities specifically cited include

(a) Data Retrieval

- Rapid, efficient retrieval from multiple files
- Ability to retrieve both quantitative and qualitative data.

(b) Data Reduction/Analysis Features to be Provided are to Include

- Statistical control of input data quality
- Hypothesis testing
- Grouping of data sets by selected parameters
- Characterization of data distributions by average performance and variability
- Functional and statistical relationship studies
- Special analyses desired by users on a non-routine basis
- Cost benefit modeling.

(c) Report Generation

- Provision for preparing standard computer generated reports.

B. IR (Decision) Model

(1) A generalized IR model is to be developed for assessment/selection of best approach for restoration, taking into account technical and economic feasibility.

(2) The IR model is (to the extent possible) to be based on existing models, such as USGS' or WES' models.

(3) IR model is to serve as the basis for integrated analysis of the data obtained in the technology base development phase, and as the means to ensure efficient use of data and to preclude duplication of R&D tasks in the IR program.

C. Data

(1) All data required or potentially required with respect to IR decisions is to be collected and retained in a centralized mode (see A.2).

(2) General priorities for collecting, organizing, and managing data area as follows:

(a) Data required for identifying migrating pollutants and their sources

(b) Data needed to establish immediacy of the threat of migrating pollutants to public health and safety

(c) Data needed to establish acceptable concentration limits

(d) Data needed to assess and select appropriate control measures on the basis of technical and economic feasibility.

(3) More specifically, data to be collected by functional area include:

(a) <u>Sampling and Analysis</u>

- Pollutants - raw data concerning the type, location, three dimensional boundary (profile), and level of pollution of soil, water, and facilities; data needed to determine whether pollutants are migrating

- Ecology - baseline data will be collected on life forms-vegetation, invertebrates, fish, mammals, birds, amphibians, reptiles - to determine the presence and potential effects of pollutants throughout the ecosystem.

(b) <u>Standards Development</u>

- Problem Definition Studies - information will be collected to identify the toxicological hazards of pollutants that occur at each installation

- Chemistry and Toxicity Studies - data to assess the risks at various concentration levels of pollutants will be gathered through literature and controlled laboratory studies.

(c) <u>Decontamination Technology Development</u>

- Through appropriate research, engineering analysis, and pilot projects, data is to be collected to enable the establishment of feasible treatment technologies.

(d) <u>Cost Benefit Modeling</u>

- Based on data resulting from the efforts above and in conjunction with computerized decision making aids, procedures for optimum selection from alternative control options are to be developed. Cost benefit models are to be used to assess (quantitatively and qualitatively) the tradeoffs in reducing contamination, costs, time and manpower.

(4) All data collection, formatting, storage, and output (i.e., report generation) will, to the extent possible, follow prescribed standards so as to be generally applicable to any installation study.

D. Users

General user groups who will be interfacing with the IR Data Manage-System include:

(1) PM-CDIR located at Edgewood Arsenal. This group will represent direct-access users of the system. It will also be serviced by EA data management and programming staff.

(2) IR personnel comprising various functional areas and stationed at active installation sites. These groups will be active suppliers of data as well as users of data.

(3) Special groups that will impact heavily the IR Technology Base Development Phase, including the Office of the Surgeon General, Analytical Systems Committee, etc.

E. Organization/Staffing/Resources

(1) The data management system development is to be contracted due to unavailability of staff within PM-CDIR. Most of the tasks have been assigned to Edgewood Arsenal.

(2) The activity is to be monitored by PM-IR out of IR/Technology Development.

(3) To ensure proper coordination of the effort, a Data Management Project Officer has been established within PM-CDIR.

(4) Development is to be coordinated with all interest groups, including PM-CDIR, installation staff, ASG, ASC, etc. The data system is to evolve through close coordination with staff representing the major IR functional areas.

(5) By PM-CDIR acceptance of the Data Management Plan (Revision 1), staffing requirements for this effort are understood to be about 7 to 8 professionals per year during FY '77 and FY '78.

(6) Budget requirements, while still in the process of being developed, are acknowledged as roughly $700,000 to $1,000,000 dollars per year.

Compliance With Policy

Battelle believes that the evolving data base is in keeping with the extracted policy of the PM-IR. Caution is noted, in that the principal behind the establishment is the same principal leading the development of the data base. While this will enhance the incorporation of established policy into the data base, it can also restrict policy implicitly by hard- or soft-ware limitations.

Policy Alternatives

In the study of this policy structure, certain discussion areas were found which could affect the policy set of the PM-IR. These are presented in an issue format, and some are also discussed later in text.

Issue Quantitative Data

Should more data of a quantitative type be added to the data management system?

Pro

The data management system is designed to capture data elements for the following groups:

- Concentration
- Quality control data
- Analytic information
- Location.

Yet, with all of the data being stored on the system, examples of further data needs abound. Several examples include:

A "sample block" identifier, to logically group samples into homogeneous zones.

A field estimate of field coefficient of variation, to supplement the laboratory estimate of laboratory COV.

A reference to a field and/or lab book, for substantiating information.

A field to note that the stored data has been checked and verified against the original data.

Con

In comparison to the contemporary environmental data bases run by the government, too much data is already stored in the data base. Further, that data which is not in the base is reported in the log books, and is largely unnecessary in modeling studies. All that is required is to be able to trace back to potentially erroneous entries.

Issue Qualitative Data

Should descriptive information be added to the central data management system?

Pro

Frequently, an observation with curious results can easily be explained with several short lines of descriptive information. Such information could readily be added to the data base, and would provide an easy means of studying outfliers without resulting to the lab and field books.

Con

Such entries cannot be processed by computer programs, and thus represent unnecessary addenda.

Issue - Non - Stored Data

The process of collecting field data involves the maintenance of field and laboratory data books. Should these be part of the central data management system?

Pro

Under an implicit policy all of the data collection efforts at the installations fall within the purview of the PM-CDIR.

Field experience at Battelle has shown field comments (and laboratory comments) to be valuable in the interpretation of results. In one instance, on observed concentration 4000 times normal values was explained by observed circumstances. Qualitative observations of interferences, mentioned in lab books but not recorded quantitatively, are also valuable in the examination of outfliers.

Future users of the stored data will suffer if they are not privy to the circumstances and rationale surrounding the taking of a sample.

Con

The users of governmental data networks (SAROAD, etc.) are not provided with these explanatory data.

The sense of ownership of collected data was expressed strongly by several installations - almost to the point of refusal to provide complete data sets to the central site. This sense of ownership will extend, perhaps even more strongly, to the lab and field books.

Without previous lab and field books at hand, future studies will be forced to proceed nearly blind of the history of accumulated qualitative experience in these data books.

Issue - Flexibility

Should the Data Management System continue to be developed, or should it become fixed at point in its development?

Pro

No one is smart enough to foresee all eventual needs and problems, therefore the Data Management System needs to either be responsive or will suffer from obsolescence.

The needs of the ultimate users of the data, those who will utilize the data to decide on restoration activities, are yet undefined. An attempt to define these needs is premature.

Con

The revision of input data to the Data Management System requires not only the revision of software at the central site, but also software at the remote sites. Further, the revision dates previously stored data, necessitating an update procedure for which data may not be available.

Management Information Systems

There exist management information systems designed to keep formal track of complex programs, and to perform accounting algorithms on each flow, personnel needs, etc., and also to compute critical paths. Should these be instituted as part of the Data Management System?

Pro

These existing programs are quite good in their operation, and could easily be built into the central site computer. Use of these systems may alleviate some of the continual pressure on IR staff, as knowledge man-power commitments can cause a decrease in the acceptance of new projects, and can also provide for a balancing and scheduling of loads. Finally, the report generators within management information systems can decrease the manual preparation of reports.

Con

Proper utilization of an MIS requires initial and continuing effort to provide for input data to the system. This workload may be higher than the time gain from its use.

DATA REQUIREMENTS

The purpose of this task was to evaluate input data requirements of the IR Data Management System, and to identify marginal or excessive data.

The data base exists to serve its customers, and thus should be designed to store any data requested of it. On the other hand, the customers of the data base have not sorted out objectives, and thus ask the data base to store all collected data. This loop can feed upon itself and cause the data base to be swamped in processing great volumes of unusable data.

It is not the responsibility of the data base manager to define needed data. Rather, it is the responsibility of site managers to assure that collected data is of value to the IR program.

Data Included Which is Excessive

This topic includes not only the elements of individual entries, but also whole categories of entries which can be considered excessive.

In reviewing the list of input elements for the data base, there was some discussion at Battelle over the value of some of the elements. It was decided that, since the data base exists, and since the stability of the system is deemed more valuable than the cost of storage, that those elements should continue to be stored.

In the process of storing data, a great volume of essentially replicative supporting data must be submitted. The use of the laboratory computes to structure input is desired. However, as the data base evolves, it's structuring will not require supporting structure for, say, each chemical analysis. A significant increase in accuracy and decrease in computer time/connect time will be realized if the laboratory computers can structure data in its assembly for transmission to the central site, avoiding the nonessential replication.

Battelle is, at this time, reserving comment on the categories of data being stored. Battelle criticized what it believed to be the most nonessential use of the data base - that of storing health standards - pointing out that such a use could be superceded inexpensively by use of a published and regularly updated document. The PM-IR countered the criticism with the concept of using the central site computer as the communication mechanism. Thus, using this philosophy, all data which is collected should be stored in the data base.

Finally, the discussion should touch upon the quality and types of information being collected in the field. As the program now exists, Battelle perceives the data collection activities proceeding as follows (especially for concentration data):

(1) Perception of problem.

(2) Sampling to determine if problem.

(3) Further sampling to define problem.

After the collection of samples, it has been discovered that basic questions remain unanswered.

Battelle does not find fault here -- the process of environmental sampling yet remains a difficult art. However, in the future, there are recommended steps which should be considered, as follows:

(1) Perception of problem.

(2) Preliminary survey to scope magnitude/bounds of problem.

(3) Documentation of sampling plan, including consideration for

   (a) Purpose of intended samples

   (b) Required support data

   (c) Blocking of sampling effort, and other questions of the statistical design

   (d) Possible effects of uncontrolled variables

   (e) Sampling (field) error estimates

   (f) Cost.

These documents should become part of the IR Data Management System. A post-sampling evaluation of the outcome of the sampling program should accompany the documents.*

The process of "thinking through" a sampling program and the resultant use of collected data will cause the resultant collected data to be of more worth to the IR program.

Data Not Included

Several elements should be added to the data base entries. These are

(1) A notation indicating the lab and field sampling book identification numbers, to aid in tracing outfliers. (Again, these books should be managed by the IR program).

(2) An entry which denotes a sampling area (a statistical block, a generic location, i.e., Yellow Lake, etc.), to aid in organizing stored data.

(3) An entry estimating the size of the field sampling "error". Much effort is given to the documentation of lab error. Similar concern, but less effort, should be given to the field (within block) variation estimates, which is smaller. This number could be estimated or priori, or calculated from the collected within block variation.

In addition to the quantitative data presently in the data base, Battelle believes the utility of the data base would be enhanced if a qualitative data field were allowed to describe special circumstances surrounding individual samples.

SYSTEM MODELING

To set the record clear at the outset, there does not now exist a comprehensive environmental model with cost/benefit analysis for cleanup alternatives in sufficient generalization to encompass the wide range of situations found at the various installations. And, at the outset such a goal appears to be an unachievable one.

However, the storage of data has two purposes. In its first use, descriptive statistics can be drawn from the collective data and used to describe the current degree of contamination, as well as to allow subjective modeling and interpolation and extrapolation of results. For this use alone, the existence of a central Data Management System can be justified.

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* This can't be stressed enough. A sampling program to "document plume profiles" has needs that differ from a program to "calibrate a plume model". Battelle perceives that most collected data has been for the former need, rather than the latter -- which leads to the expressed question of whether too much data have been collected. Certainly, a case can be made that too much data has been collected for some areas at some sites (for descriptive purposes). This could have been averted by paying attention to the required accuracy of the descriptive statistics.

The question addressed here is whether system modeling is needed in the IR program. Clearly, a discuss of which "system modeling" is to be required. Based upon the perceptions we have, the decision model is to

(1) Simulate existing contamination at a given installation.

(2) Extrapolate future contamination patterns at that installation for various cleanup options.

(3) Determine the cost of the cleanup options.

(4) Assess a measure of worth of cleanup, so that cost/benefit ratios can be calculated.

There is an incorrect tendency to interpret the decision model as a totally integrated software system which will spit out conclusive, optimum answers with respect to control alternatives. Rather, the system might better be viewed (initially) as an array of software modules, linked to data files, that are executed in a more iterative fashion requiring step-by-step analysis. While certain portions of the model may be quite sensitive and accurate, other components may be much more primitive and subject to qualitative interpretation.

The model(s) should perhaps be viewed as a rigorous scheme for organizing and analyzing the large mass of data that are generated by the various functional areas (i.e., sampling and analysis, standards, decontamination technology, and cost/benefit data). In some sense, attempts to fully define the data variables that the DMS is to handle prior to defining the model(s) to be developed are premature. Since data to be collected represent inputs, the model(s) must dictate the type of data needed.

Of the functions described, the process of contaminant modeling, and of defining benefits, are not well defined. Toward the latter, the EPA has spent large sums of money to quantify benefits of air pollution control, to no avail. The PM-IR will likely have to devise ad hoc measures of benefits, such as

- Percentage of migration below standard
- Maximum concentration of migrating contaminant
- Etc.

While such measures cannot be used to justify the mission of the IR program, they can be used in a classical cost-benefit sense to select the ultimate choice of cleanup alternative.

Toward the former, the mission of PM-CDIR is not to develop the best models possible. Rather, the PM will use existing, relatively simple models trying to describe, in a first order sense, the relationships between contamination and environment. Model precision would be required only when modeled results are about equivalent to standards.

The information from models is informative and will be used in guidling the decision making process. For example, there exist complicated models for the flow of contaminated groundwater, yet the U.S.G.S. applied a relatively simple 3-dof model at RMA, with perhaps the following rationale.

(1) Sufficient spatial detail wasn't available to support a more complicated model.

(2) Uncertainties in the physical properties of the contaminants as they affect soil passage argued against a more complicated model.

The results of this modeling exercise demonstrated that contamination currently exceeds the interim standards at many off-base locations, and will continue to do so, if unabated, into the long term future.

The significant point of the exercise, however, is that the modeled contaminant concentrations were on a scale too coarse to permit the actual phased design which occurred. Thus, the design used actual current data and, where necessary, much simpler models, rather than the more sophisticated but less detailed U.S.G.S. model results.

This situation is most likely to occur in other migration problems faced by the PM-CDIR. Where sophisticated models are available, future projections could point to continuing migration problems. However, the mission of the PM is to "stop migrating contaminants", and not "assure the migration will eventually cease". Hence the most likely approach of PM staff will be to employ simple models which address the former, rather than sophisticated models which address the latter.

For this purpose, a list of accepted transport and diffusion models has been prepared. Generally speaking, several years of aerometric data are desired for long-term modeling purposes, but these can be procured from nearby airport stations. Thus an intensive data collection effort for atmospheric emissions is probably not justified.

DIFFUSION MODELS FOR ASSESSMENT OF AIR QUALITY IMPACTS

A number of diffusion models can be used in assessing air quality impacts associated with emissions from point, area, and line sources. These models will be presented in this discussion. As the number of sources, number of pollutants (reactive and nonreactive), and the size and complexity of study regions increase, air pollution modeling capabilities have responded to current and future assessment needs. Thus, atmospheric dispersion models have become available with varying degrees of sophistication and flexibility. This discussion will present the capabilities and intended usages of each model.

Diffusion models are a mathematical tool which simulate the various meteorological processes that affect airborne effluents from a pollutant source or a group of sources. More specifically, diffusion models aid in analyzing and predicting the spatial concentration distribution of a pollutant and describe any distribution changes that may occur from projected variation in source strengths.

The most common technique in mathematically describing the spread of the plume from a source and the approach used in most of the models discussed is the Gaussian diffusion formulation. This approach stems from the fact that the well-known normal, or Gaussian distribution function provides a fundamental solution to the classic Fickian diffusion equation.[1] In a Gaussian plume model, the crosswind plume concentration distributions are assumed to follow a normal distribution (Gaussian). This has been partially substantiated from field experimental data for typical meteorological conditions and for averaging times of 1 hour or longer. The Gaussian diffusion model is valid only for long diffusion times and for homogeneous stationary conditions. However, this type of model has been found to give useful results for many practical applications. Unless otherwise indicated, all of the models discussed herein are steady-state Gaussian plume models. Steady-state implies that concentrations are not time-dependent in the normal sense; that is, input variables such as wind direction and wind speed are updated, at best, once per hour.

The presentation of the mathematical models is arranged according to the type of emission source being assessed and according to pollutant for which the model is valid. The various types of emission sources are point (usually a stack), area, and line (i.e., usually a roadway) source. Several models have been created which consider specific pollutants such as carbon monoxide and photochemical oxidants.

Point Source Models

EPA Models

The three point source models listed below are available on the UNAMAP tape disc. This tape also includes three other models: CDM, HIWAY, and APRAC.(2) The "Valley" and "CRSTER" point source models and the "RAM" urban diffusion model are presently being placed on the UNAMAP tape by the Environmental Protection Agency. The UNAMAP tape can be purchased from the EPA. User's manuals for each model are included in the purchase price. These manuals provide description, operation, and execution instructions.

PTDIS. A steady-state Gaussian plume point source model that calculates ground level concentrations for various downwind distances. The user can specify a maximum of 50 distances. The model considers only one source for a single meteorological condition.

PTMAX. A steady-state Gaussian plume point source model which is primarily used in determining the wind speed and atmospheric stability that will cause the maximum concentration for a given source. Like PTDIS, separate computer runs are required for each point source. The results of PTMAX are indirectly used as input into more sophisticated models such as AQDM and CDM.

PTMTP. A steady-state Gaussian plume point source model that computes hourly pollutant concentrations at a maximum of 30 receptors for as many as 25 point sources. This model is applicable to assessing the air quality impact from multiple point sources.

The models discussed above do not evaluate terrain heights. Concentrations are estimated assuming a flat terrain. The following two dispersion models do consider terrain heights. The "Valley" model was created primarily to evaluate terrain height differences between source and receptor.

CRSTR.[3] A dispersion model which has been proposed by U.S. EPA as the preferred prediction model for determining the maximum short-term concentrations produced by an individual point source such as a power plant.[4] It calculates maximum daily pollutant concentration, identifies the meteorological conditions responsible for the maximum and calculates hourly concentrations for an entire year at an array of receptor locations. The concentrations are calculated for 180 receptor locations situated at each of 36 cardinal directions from the source and at five different distances. The model handles from 1 to 19 sources but assumes all are at the same physical location.

Valley. A dispersion model which predicts both short-term (24-hour) and long-term (annual, seasonal) pollutant concentrations in an uneven terrain. Sources at only one location are considered. Eighty receptors are predefined in 16 cardinal wind directions (five in each direction) about the source. The user specifies the distance interval separating the receptors. Required meteorological data consist of a wind distribution by stability class for either long term or short term.

Area Source Models

Non-EPA Models

Rollback Model.[5] The rollback model does not consider the dispersion of pollutants from a source; rather it is a technique which is the simplest method used in determining the emission reduction needed to attain an air quality standard for an area or point source. The rollback method is represented by the following proportion equation:

$$\frac{A-C}{A-B} \times 100 = \text{percent reduction needed}$$

where

A = existing air quality at the location having the highest measured or estimated concentration in the region

B = background concentration

C = national standard.

Since there is no allowance for specifying meteorological parameters, this technique cannot be used to estimate concentrations at sites where representative air quality data are not available.

Miller-Holzworth.[6] This dispersion model is a step in sophistication above the rollback model. The model can be used to estimate a 1-hour integrated area-wide average pollutant concentration (TSP, SO_2) for the area under consideration. Unlike the rollback model, the model can be used for an area where no air quality data are available. This is because atmospheric dispersion is accounted for in the model.

Hanna-Gifford.[7] This model is applicable for areas where there is no point source information available. Emissions are therefore grouped into area source emissions. The Hanna-Gifford model is used to estimate 1-hour and annual average concentrations of stable pollutants such as sulfur dioxide, particulates, and carbon monoxide. It differs from the two previous models in that it accounts for the dispersion constant, K, which is a function of atmospheric stability and distance. (This model is available from Steve Hanna of the National Oceanic and Atmospheric Administration in Oak Ridge, Tennessee.)

Line Source Models

EPA Models

HIWAY.[2] A basic line source dispersion model. It is applicable to mobile source pollutant emissions along streets and highways and is valid only for pollutant emissions (CO and fine particulate matter) from automotive sources. HIWAY calculates only 1-hour average concentrations of these pollutants.

Non-EPA Models

CALINE.[2] The California Line Source Model is also a line source model whose capabilities match HIWAY. However, it is believed that CALINE is more accurate in its predictions of concentrations in cut and fill sections of a highway. (CALINE highway diffusion model is available through the California Transportation Department.)

Point and Area Source Models

EPA Models

AQDM--Air Quality Display Model.[8] A long-term urban dispersion model which is best used to determine annual average concentration of SO_2 and TSP. The model is applied to areas with numerous point and area sources. AQDM can be used to estimate concentrations at any downwind point (receptor). Basic input includes a comprehensive emissions inventory of point and area sources and a joint frequency distribution of wind speed (six classes), wind direction (16 cardinal points), and stability classes (Pasquill classes).

CDM--Climatological Dispersion Model.[2,9] An urban Gaussian dispersion model that estimates short- and long-term (24-hour) annual pollutant concentrations (particulate, sulfur dioxide) for any combination of point and area sources. Its capabilities and applications are similar to AQDM. However, the manner in which CDM determines concentrations from area sources is different and CDM uses an empirical power law function to determine the wind profile. CDM's prediction of concentration is believed to be more accurate than AQDM's.

RAM.[10] This is a short-term (1-hour to 1-day) steady-state, Gaussian diffusion model for estimating air quality concentrations from point and area sources. RAM has several uses.

Effects of either control strategies or tactics for specific short-term periods may be examined by users. The expected effect of a proposed source or sources can also be determined. The spatial variation in air quality throughout the urban area or in a portion of the area for specific periods can be estimated. In a forecast or predictive mode such as over a 24-hour period, the algorithm can assist in placing mobile or portable air samplers and in developing emission reduction tactics. Its success in the forecast mode is contingent on the validity of the algorithm assumptions and on the accuracy of both the input meteorological parameter values and the input emission parameter values.

There are, however, several limitations in applying this model. These limitations are common for all steady-state Gaussian diffusion models.

Computations are performed hour by hour as if the atmosphere has achieved a steady-state condition. Therefore, errors will occur where there is a gradual build-up (or decrease) in concentrations from hour to hour, such as with light wind conditions. Also, under light wind conditions, definition of wind direction is likely to be inaccurate and variations in the wind flow from location to location in the area are quite probable.

RAM is not appropriate for making concentration estimates where there are topographic complications. The greater the departure from relatively flat terrain conditions, the greater the departure from the assumptions of the algorithm.

RAM is most applicable for pollutants that are quite stable chemically and physically. A general loss of pollutant with time can be accounted for by the model. However, it is poor at handling cases when there is selective removal or reaction at the plume-ground interface or when the removal or reaction is dependent upon pollutant concentration levels.

The higher the physical and resulting effective heights of point sources, the greater the chance for poorer results since actual directional shear in the atmosphere, which is not included in the algorithm, will cause plumes to move in directions different from the direction input to the model. Also, the higher the source height, the greater the potential for encountering layers in the atmosphere having dispersion characteristics different from that being used.

Non-EPA Models

TCM--Texas Climatological Model.[11] An urban Gaussian dispersion model that estimates short- (24-hour) and long-term (annual) pollutant concentrations (particulate, sulfur dioxide) for any combination of point and area sources. This model, available through the Texas Air Control Board in Austin, Texas, is primarily the Climatological Dispersion Model (CDM) with several major modifications. One, TCM solves the dispersion equation by interpolating in a table of precalculated coefficients, rather than the time-consuming explicit calculations of the exponentials involved. Thus, computer running time for the TCM model is much shorter than for the CDM. This is the primary feature of the TCM model. Second, concentrations from area sources are determined using the Hanna-Gifford approach. This also contributes to the reduced running time of the TCM. One important note, however, is that the Texas Climatological Model with its approximations is most applicable to the large metropolitan cities in Texas whose emission inventories are characterized by a small percentage of area sources. The model is most reliable in urban areas where approximately 90 percent of the sources are point sources and the remaining 10 percent are area sources.

TEM--Texas Episodic Model.[12] This model, developed by the Texas Air Control Board in Austin, Texas, is the short-term companion of the TCM. Its structure is almost identical to TCM with emphasis on short-term concentrations. This model has been used by the Texas Air Control Board to identify trouble spots in its air quality maintenance areas and aid in formulating control strategies. TEM is used routinely by the TACB's Permit Section in analyzing new construction permit applications from Texas industries.

SAI. A photochemical dispersion model. This model estimates hourly concentration variations of these pollutants: CO, HC, NO, NO_2, and oxidant. It not only considers the transport and dispersion of these pollutants but also the transformation of HC and nitrogen oxides into photochemical oxidant pollutants. SAI is not a Gaussian-formulated model. Instead, this model uses finite difference techniques over a grid of area sources to solve the classical equations of mass conservation which include local changes, advection, diffusion, photochemical reaction, and emission.

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WATER QUALITY AND WATER RUNOFF MODELS FOR ASSESSMENT OF WATER POLLUTION IMPACTS

Water quality models play an important role in the assessment of water pollutant transport in surface waters, the design of alternative waste abatement measures, and the evaluation of alternative water quality management programs. Water quality in a given waterway is a function of a number of biological, chemical, physical, and hydrological factors. To determine the combined effort of these various factors, water quality models have been developed in various degrees of sophistication and flexibility.

Water quality models may be distinguished by the types of water quality constituents (conservative or nonconservative), waterways (rivers, lakes, impoundment, or estuaries), or sources of pollution (point or non-point) simulated. This discussion will present various water quality models capable of simulating any combination of the above types.

Water Quality Models

EPA Models

AUTO-QUAL.[1] Is designed specifically to simulate fully-mixed bodies of water where widths are small relative to their lengths such as freshwater streams and tidal tributaries to estuarine bays. A two-part model, it can simulate steady-state, as well as, time-dependent concentrations for carbonaceous and nitrogenous BOD and DO. However, the hydraulic solution for both parts of this model represents a net, steady-state situation. Thus, tidal flow, storm surges, or any other unsteady flow condition are not considered by this model. There is both a steady-state and dynamic version of this model.

Non-EPA Models

QUAL-1.[2,3] This steady-state model simulates spatial and temporal variations of biochemical oxygen demand, dissolved oxygen, temperature, and as many as three conservative minerals* (such as total dissolved solids, chloride, and sulfide) within a one-dimensional, fully mixed, branching stream or canal system. Major transport mechanisms, advection and dispersion, are assumed only along the longitudinal axis of the stream or canal. It allows up to a maximum of 25 waste discharges and water withdrawals, five tributary flows, and five headwaters. Also, it has the capability of calculating required dilution flows for flow augmentation to meet any specified dissolved oxygen level.

QUAL-2.[4] Is a modified version of QUAL-1 to include the following improvements over the original model:

- Capability to simulate steady-state temperature
- Capability to dynamically simulate water-quality parameters
- Capability to input initial conditions for dynamic simulation in a continuous manner
- Capability to operate in metric units.

The parameters modeled are: chlorophyll, a nitrogen (ammonia, nitrite, nitrate), phosphorus, carbonaceous BOD, benthic oxygen demand, dissolved oxygen, coliforms, radioactive material, and conservative substances. The basic difference between QUAL-1 and QUAL-2 is that the latter can solve steady-state problems plus it includes complex reactions and interactions such as nutrient cycles and algae production for the simulation of its nonconservative parameters. This model allows up to a maximum of 15 headwaters, 15 tributary flows, and 90 input and withdrawal elements.

DOSAG-1.[5] Is used to simulate spatial and temporal variations in BOD and DO under various conditions of temperature and headwater flow.

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* A conservative mineral is one that is assumed to have no sources or sinks other than local inflows or diversions.

This program was designed to be used as a compliment to QUAL-1 since it allows rapid evaluation of a number of varying stream conditions. Since the program was designed to be run for varying climatic and hydrologic conditions during a 12-month period, it is possible to input up to 12 different temperatures and corresponding discharges to each of the headwaters within the stream system modeled. In general, this model provides a general description of the DO sources of the stream system modeled, as well as the required flow augmentation to bring the system up to the required target level DO concentration. Also, it has the capability to find the DO distributions for varying levels of treatment (waste treatment plants) in the simulated stream. It allows up to a maximum of 20 tributary flows, 10 headwaters, four DO target levels, and five degrees of treatment for both carbonaceous and nitrogenous wastes. Large impoundments such as reservoirs are not considered by this model.

RECEIV-II.[6] This model was developed by Raytheon Company for the U.S. EPA by modifying the Receiving Water Block (RECEIV) of the U.S. EPA's Storm Water Management Model (SWMM). This time-varying, two-dimensional model has the capability of simulating a wide variety of waterways ranging from upland streams through shallow lakes and impoundments to estuaries. It is best suited for estuaries. Also, it has the capability of simulating concentrations for 11 water quality parameters considering any interactions among them. These parameters are: phosphorous, coliforms, ammonia nitrogen, nitrate, nitrite, total nitrogen, BOD, chlorophyll a, salinity, and one nonconservative metal ion. Because of its dynamic condition, the model is recommended for the simulation of estuaries, for use in cases of unsteady discharge such as runoff, for extrapolation to low-flow conditions, and for evaluation of seasonal, tidal, or daily variations in water quality.

EXPLORE-1.[7,8] This model, developed by Baca, et al.[8], simulates hydrodynamics and water quality dynamics for rivers, well-mixed estuaries (including tidal influences), and thermally stratified reservoirs. A pseudo two-dimensional approach is used to formulate hydraulics and mass transport. Water quality parameters which can be predicted with this model are: nitrogen (total ammonia, nitrate, nitrite), phosphorous, salinity, BOD, DO, solphite waste liquor, a toxic compound, chlorophyll a, and coliforms. This model contains a momentum balance which permits flood routing during storm events. The capability of simulating tide flat areas which may dry up at low tide is available through this model.

NPS.[9] The Nonpoint Source Pollutant Loading (NPS) model is a continuous simulation model that represents the generation of nonpoint source pollutants from the land surface. It simulates hydrologic processes (surface and subsurface), snow accumulation and melt, sediment generation, pollutant accumulation and pollutant transport for any specified period of meteorologic data input. The model can accommodate up to five land-use categories and simulates water temperature, DO, sediment, suspended solids, and up to five user-specified partially-soluble pollutants (nutrients, heavy metals, etc.) for each land use. Since the model does not simulate channel processes, modeling should be restricted to watersheds smaller than 2 square miles. Thus, to simulate in-stream water quality in larger watersheds, the model must be interfaced with one that simulates channel processes.

PIONEER.[7] Is a steady-state model which simulates rivers (or portions of rivers) free of tidal influence. It has the capability to model large basins with many point and nonpoint pollution sources. This model is set up to handle the same pollutants as EXPLORE-1.

DEM.[9] Simulates the unsteady flow and dispersional characteristics of both conservative and nonconservative water quality parameters in a nonstratified estuary. The Pearl Harbor version of this model incorporates the heat budget heat terms of the "Tidal Temperature Model" and expands the DEM by means of QUAL-2 to include up to 15 different specified parameters. These parameters are: temperature, DO, BOD, chlorophyll a, nitrogen (ammonia, nitrite, nitrate, total), phosphate phosphorous, coliforms, total dissolved solids, two heavy metals, and two pesticides. Time and space scales in this model should approximate as nearly as possible the physical, tidal, and climatic characteristics of the system modeled. The model can simulate as many as 200 junctions, 400 channels, and seven tidal coefficients.

reaeration coefficient and thus the dissolved oxygen levels in the stream. Computations made with SWOHS show that the hydraulic effect is likely to be minimal in all except the most extreme cases.

Pesticide-Insecticide Water Runoff Models

EPA Models

ARM--Agricultural Runoff Model.[13] ARM is a continuous simulation runoff model which simulates pesticide and nutrient loads to stream channels from both surface and subsurface sources. No channel routing procedures are included. Thus, the model is applicable to watersheds that are small enough that channel processes and transformations can be assumed negligible. Although the limiting area will vary with climatic and topographic characteristics, watersheds greater than 1-2 square miles are approaching the upper limit of applicability of the ARM. This model can be obtained through the EPA.

Non-EPA Models

FETRA--Finite Element Sediment and Contaminant Transport Model.[14,15] A modified version of the SEDATRA[14] model, FETRA is capable of simulating time-dependent, laterial, and longitudinal distributions of sediment and pesticide concentrations within a particular body of water. It takes into account sediment-pesticide interactions. Steady-state predictions are also possible with this model. The considerable amount of data input which may or may not be readily available is the major drawback of this model. The data include: information on depth variations of the waterway, flow characteristics, size distribution of suspended and bed sediments, suspended sediment load, critical shear stresses for cohesive sediment erosion and deposition, erodibility coefficients, initial distribution of the pesticide in bottom sediments, initial pesticide concentrations in dissolved and particulate phases, and pesticide distribution coefficients between sediment and water. In addition to pesticides, this model can be used to model any other pollutant which is transported in the dissolved state, and absorbed by suspended and bed sediments.

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GROUND-WATER MODELS FOR ASSESSMENT OF POLLUTANT MIGRATION AND DESIGN OF CONTROL MEASURES

The models needed for assessment of the migration of pollutants in ground-water aquifers and for evaluation of the design of control measures are discussed. These models are available with varying degrees of sophistication, documentation, and flexibility. Thus, models can be selected that fit the complexity of a particular problem and the amount and accuracy of known geohydrologic data. When these models are applied to a particular problem and the necessary input parameters are known with sufficient accuracy, measures for controlling the spread of contaminants in an aquifer system (by pumping, treatment, and injection) can be designed with a factor of 2 to 3. The control measures can then be installed in increments to obtain the correction factor needed to adequately size the pumping, treatment, and injection facilities. The effects of other corrective measures such as surface sealing and slurry walls can also be evaluated using these models.

The use of ground-water modeling as a water management tool has developed rapidly over recent years. Models have been used on many different types of problems which include: (1) ground-water flow in saturated or unsaturated materials, (2) land subsidence associated with dewatering, (3) flow in coupled ground-water stream systems, (4) rainfall-runoff coupled with soil moisture and ground-water flow in small watersheds, (5) interaction of economic and hydrologic considerations, (6) predicting the transport of pollutants, and (7) estimating the effects of proposed development schemes for geothermal systems.[1] These models are in continued stages of development. However, adequate model development has already been accomplished to apply these models to the solution of problems involving ground-water transport of pollutants.

Pollutants usually enter the ground-water system from (1) surface spills, (2) seepage from holding ponds, (3) leaching of buried waste, and (4) deep-well injection. In the first three modes of pollutant entry to the ground-water system, flow is usually through the unsaturated zone prior to its entry into the saturated ground-water zone. In problems of this nature, both saturated and unsaturated ground-water flow must be modeled to obtain the flow data necessary for predicting ground-water transport of pollutants. In all of these cases of surface or near-surface release of pollutants, precipitation plays a major role in the rate of pollutant migration. Therefore, in humid regions, the consideration of rainfall-runoff and its coupling to soil moisture (the unsaturated zone) must be considered. In arid regions or in confined aquifers, the unsaturated zone and the effects of precipitation can usually be neglected.

Ground-water models are used to obtain the water flow (velocity) data in the region under investigation. These velocity data are then used as input to pollutant transport models which predict the concentration of pollutants at various points of interest in the region. Thus, for prediction of ground-water transport, a detailed understanding of the water flow system is required; and the accuracy of the predictions of pollutant concentration relate directly to the accuracy of the ground-water flow simulation. For the simulation, flow and transport, both physical and chemical properties of the aquifer system are required. The parameters that describe these aquifer properties are:

- Flow parameters (saturated)
  - Transmissivity - hydraulic conductivity times saturated thickness
  - Storage coefficients - specific storage times saturated thickness, where specific storage contains both the compressibility of water and the solid medium
  - Effective porosity
  - Pumping and injection rates
- Flow parameters (unsaturated)
  - Relationship between hydraulic conductivity and pressure
  - Relationship between moisture content and pressure
  - Effective porosity
  - Modified coefficient of compressibility of the medium

transport case should be considered first. In saturated-unsaturated systems, the two-dimensions will form a cross section through the aquifer and in saturated systems either a cross section or two horizontal dimensions can be considered. However, many transport problems are truly three-dimensional and can only be simulated using models that provide solutions in three space dimensions. A few three-dimensional models are available; however, aquifer parameters in this detail are usually not available and can only be obtained through intensive field investigations. For this reason, it is best to begin the analysis with simple models and progress toward more complex models until the desired level of resolution is reached. In this way, on many problems, the investigator may reach the desired level of resolution without the expense of obtaining the parameters required for a fully three-dimensional analysis.

In the following sections, only models adequate for assessment of the design of control measures will be discussed. The discussion of models that follows will be devoted to two- and three-dimensional models where numerical methods are used in the solution of the ground-water flow and transport equations. These models have enough flexibility so that they can be applied to most ground-water problems without extensive modification of the existing computer codes. The topics covered are ground-water flow models, models for solution of the inverse problem, and ground-water transport models.

The ground-water models that are presented in this discussion are not available through the Environmental Protection Agency. To procure copies of these models, the authors of a particular model should be contacted. Mailing addresses are given for some of the authors.

Ground-Water Flow Models

Because of the flexibility in using finite element methods for the solution of ground-water problems, the models discussed in this and following sections are primarily finite element models. The finite element method allows the investigator to input different material properties in different regions of the aquifer system and to better fit the boundaries

- Modified coefficient of compressibility of water
- Precipitation, pumping, or injection rates
- Transport parameters
  - Components of dispersivity
  - Bulk density of the medium
  - Effective porosity
  - Distribution coefficient (linear sorption)
  - Decay rate (linear), if any
  - Components of fluid flow
  - Initial source concentration.

All of the parameters can vary within an aquifer system based on changes in mineralogy, lithology, and water quality. Various levels of sophistication of flow and transport models are used to account for these changes in parameters and the level of sophistication is dependent on the detail in which parameters are available in a given ground-water system. For detailed analysis of a ground-water system, the models used must be capable of simulating flow and transport through layered formations where the inhomogeneities in the formation are considered. This level of analysis requires that the parameters, listed above, be available on all of the major geologic and lithologic units in the aquifer system (within the region of interest). Usually this detailed knowledge of the aquifer system is not readily available and either a massive field investigation must be initiated or simplified (less accurate) models must be used for the evaluation of pollutant transport and proposed control measures.

In any investigation of ground-water flow and pollutant transport, it is best to begin with simple models which require the least data input. These simple models usually consist of analytical solutions to the flow and transport equations where the medium is considered to be homogeneous. Analysis of the system using simple models will provide insight into the actual flow system as well as an indication of the amount of field data that must be obtained for more detailed analysis. When more data are available, inhomogeneities can be considered using models that provide numerical solutions to the flow and transport equations. Because of the expense involved with large numerical simulations, the two-dimensional flow and of the region under consideration. Thus, an irregular boundary can be simulated easily, and layering, lenses, and other inhomogenities can be considered. This flexibility is available because each element forming the grid network of the region under consideration can have different material properties and the elements need not be rectangular or have equal dimensions.

Also, the models discussed will be applicable to flow problems in free-surface aquifers and in saturated-unsaturated ground-water systems which include the unsaturated zone as well as the free-surface aquifer. These types of models can be used in the investigation of flow through surface and near-surface disposal areas to generate the fluid flux data required for ground-water transport models.

The models discussed provide a basis for simulation of ground-water flow and transport in free-surface aquifers. They are only a small portion of the available models and represent models that have been more widely used by known researchers in the field of ground-water modeling.

FREESURF I and II[2,3]

These models were developed by Shlomo Neuman and Paul Witherspoon in 1970 and 1971 and consider steady-state and unsteady free-surface flow, respectively. They have been used to analyze flow along a vertical cross section and are limited to analysis along a cross section unless radial symmetry is assumed. The models can be used in anisotropic porous media where the region under consideration is divided into triangular and quadrilateral finite elements.

No Model Name

A two-dimensional transient model for analysis of free-surface aquifers, where material properties are averaged over the vertical dimension and flow in two horizontal dimensions is considered, was developed by George Pinder and Emil Frind.[4] This finite element model considers transient flow through an anisotropic aquifer and is versatile enough to be applied to many existing ground-water problems. (This model can be obtained from George Pinder at Princeton University or Emil Frind at the University of Waterloo.)

A finite difference model for two-dimensional flow in isotropic water table aquifers was developed by George Pinder and John Bredehoeft.[5,6] The model considers transient flow in two horizontal dimensions and material properties are averaged over the vertical dimension. (The model can be obtained from USGS or George Pinder, Princeton University.)

A three-dimensional transient or steady-state model using finite element methods was developed by P. France.[7] This model is applicable to flow problems in free-surface aquifers and would be quite useful in examination of alluvial aquifers of anisotropic nature. However, the availability of the computer code is not presently known.

A two-dimensional transient finite element model for saturated-unsaturated ground-water flow was developed in 1975.[8] This model is flexible enough to handle most ground-water problems in humid regions and uses precipitation as the surface boundary condition. One drawback is that the model can only be applied on a vertical cross section. (A user's manual for this model can be obtained from the U.S. Department of Commerce. An address is given in Reference 22.)

MOC

This finite difference model, developed by Leonard Konikow and John Bredehoeft, computes transient ground-water flow in two horizontal space dimensions. A second portion of the model uses the flow data to calculate solute transport by convection and dispersion using the method of characteristics. However, no sorption of pollutants is considered.[9] A version of this model has been used to assess pollutant migration at the Rocky Mountain Arsenal.[10]

Solution of the Inverse Problem

The inverse problem for saturated flow may be stated as follows: the fluctuations of the ground-water table over time and both the maximum and minimum water table elevations are known; aquifer recharge and discharge is known; and the ground-water flow equations are solved for the storage coefficient and transmissivity as a function of location in the aquifer. The advantage of solving the inverse problem is that water table data, infiltration, pumpage, and natural discharge are relatively easy to measure and the solution provides two parameters that are rather difficult to measure. The solution of the inverse problem can be used to guide field investigations (location of areas where aquifer tests should be conducted to measure storage coefficient and transmissivity). By combining the results of the solution of the inverse problem with existing data on aquifer parameters, the number of wells required to obtain adequate parameters for simulation of ground-water transport of pollutants can be reduced. Examples of the solution of the inverse problem are presented by Emsellem and DeMarsily(11), Neuman(12), Frind and Pinder(13), Nutbrown(14), and Chang and Yeh(15). The availability of computer codes for solution of the inverse problem has not been investigated by the author. However, development of these types of computer codes is under way in the U.S. Geological Survey and the results of the use of finite element methods for solution of the inverse problem should be available soon.

As yet, no solution of the inverse problem for ground-water transport has even been obtained. Thus, the coefficient of dispersion must still be either estimated or calculated from the results of tracer tests.

Ground-Water Transport Models

Research in the area of ground-water transport of pollutants has not been of interest to the ground-water modeler until recent years. For this reason and because the chemical reactions of pollutants in the ground are not well known, fewer ground-water transport models are available. All of the models discussed in this section are inadequate for investigation of the combined problem of pollutant transport in a free-surface aquifer and the transport from the land surface to the water table. While these problems can be studied independently, the appropriate models still have to be coupled together to analyze the vertical transport through the unsaturated zone with subsequent horizontal transport below the water table using a single model.

MOC[9,10]

MOC is a two-dimensional flow and transport model, discussed under ground-water flow models.

ISOQUAD[16]

This model uses finite element methods to solve both the ground-water flow and transport equations in two horizontal dimensions. No sorption of pollutants is considered. However, the model produced good results on the ground-water transport of chromium on Long Island, New York.

TRANSAT[17]

This model is a two-dimensional finite element model for saturated flow and transport in horizontal directions. The model can be applied to studies of ground-water contamination from waste disposal sites.

No Model Name

A two-dimensionsal finite element model for transient transport in saturated-unsaturated porous media was developed by James Duguid and Mark Reeves.[18] This model is fully compatible with their saturated-unsaturated flow model. It only applies to transport through sorbing media along a cross section. However, a second version of the model that considers horizontal flow and transport below the water table (no consideration of the unsaturated zone) has been developed and is currently operational.[19] (A user's manual can be obtained from an address indicated in Reference 22.)

A three-dimensional finite element code for simulation of both flow and transport was developed by Sumant Gupta[20] and has been applied to pollutant transport over all of Long Island. The model considers lenses and multilayered aquifers and is probably one of the most versatile ground-water models available.

A model for analytical solution of both flow and transport through the unsaturated zone was developed by Nancy Larson and Mark Reeves.[21] This model provides an approximate solution for pollutant transport through layered soils and pollutant sorption is considered. (A user's manual can be obtained from the mailing address indicated in Reference 22.)

Discussion

For investigations of most problems of ground-water pollution from surface or near-surface disposal of pollutants, adequate models are currently available. However, no single model is available that will simulate ground-water flow and tranport through both the unsaturated zone and a free surface aquifer covering a large area. The models that currently exist could be coupled at the water table to provide a single model for investigation of saturated-unsaturated ground-water problems. This modification of models would take considerable effort; however, the cost involved in model modification would not be as large as the cost involved for obtaining the hydrogeologic data and parameters for investigation of a particular problem. Many simulations of ground-water pollution have been conducted using the uncoupled systems of models and this mode of approach appears to give adequate results. It is the author's opinion that even better results could be obtained with a quasi three-dimensional model that would result from coupling an existing unsaturated model to a free surface aquifer model at the water table.

References (Ground-Water Models)

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(22) Reports and user's manual for the three models indicated can be obtained from the following address:

National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

Ecological Models

There are models available which simulate, for a specific ecosystem and a specific contaminant, the dispersion of the contaminate through a closed ecosystem. Some of these programs were developed under the NSF-RANN program for heavy metals in the environment, and some for the EPA OTS. These models are not documented here for the following reasons:

(1) The models are specific to a contaminant, and cannot be generalized to other contaminants without coefficients which are difficult to obtain through other than empirical, expensive techniques.

(2) The models are generally not applicable to an open ecosystem, such is found at all installations.

(3) A more cost effective method of obtaining ecosystem results may be had through model ecosystems, rather than computer models, for the contaminants in the IR program.

Impact of Models on IR Program

In general, in comparing the existing models with IR data collection activities, it appears that there are oversights in the data collection activities which can be improved. These oversights include:

- The lack of data to support surface runoff studies, including soil permeability, slope, cover, etc.
- The lack of data to support air dispersion studies for fugitive dust. Most of these data can be had from WOAA, but some information may be required on ground cover, etc. This is not a generally well understood area.

SYSTEM ANALYSIS

In this section, the adequacy and compatibility of hardware, and software of the Data Management System were to be assessed. However, when the study had begun, the major hardware and software decisions had been made. The 1108 Univac at EA will be employed, and the Data Manager has arranged for a reasonably optimum configuration (i.e., arrangement for removal disk packs). The MRI System 2K was a free good, and will be used. Remote site Tektronics terminals and necessary MODEMS have been purchased. However, there are some observations which are worth sharing.

Error Introduction

The significant time required to transmit remote site information over phone lines will result in the reception at the central site of some errors. Predilections of people being such as they are, it will be difficult to spend an hour echo-checking data which took hundreds of hours to generate. The use of a check-sum generation and check technique is highly recommended.

Field Variation

As mentioned before, the analytic error, which is determined and provided with each data point, is a small part of the total data variation. A field variation component should be estimated and provided with each sample.

System Stability

Each time the central data base changes its field definitions or needs to occur at remote sites. Future changes should attempt to be compatible with existing formats. Additional or altered fields should be provided on additional (but unrequired) input records. The central site should have the responsibility for updating old records.

Structured Input

To reduce connect time and data transfer needs, the data base should be formatted to receive structured data, without replicative and unnecessary fields. While it can be argued that such a capability could be provided by the programmer's at remote sites, it is likely that the Data Manager is more capable of understanding and interfacing the data base to structured data.

QC

A fairly strong laboratory quality control program is established by the PM-IR. While this activity is not within data management scope, its integral importance requires a statement as to its perceived weakness. Simply put, there are unresolved differences in the application of the quality control algorithm selected by the Q.C. committee. Further, there are erroneous assumptions in the Q.C. algorithm which cause questions in the absolute value of the "detectable limit". The Q.C. committee should resolve the differences of application, to assure commonality between sites. Further, a well trained statistician should determine whether the false assumptions of the selected technique seriously impact the estimate of detection limits.

RESEARCH REQUIREMENTS

This section is devoted to the estimation of resources required to support the suggested changes in the data management activities. Costs are estimated only for significant changes.

Addition of Fields for "Block" Qualitative Data, and Field Error

The major problem in this activity is that of appending fields to input records which are already "full". If the input records were completely restructured to allow structured input, this activity would be modest.

It is estimated that input restructuring would require about 3 man-months of activity at the central site. Done carefully, current input records could be accepted while also allowing the structured format. Thus, remote site costs could be minimal.

For the rest of this study, it is presumed that restructuring is done.

Non-Stored Data

This task would set up and maintain a library of lab and field books. Such an activity could be accomplished with less than a half man-month initial cost, plus a continuing cost of 1/10 man-year per year.

The task may be difficult to accomplish because of site management reluctance. Such reluctance could require time from the PM-IR to reduce the conflict.

Management Information Systems

This activity could be quite expensive. In addition to the purchase price of an MIS ($10,000 or more), a large effort may be required to support its input needs. Initial costs of up to 1/2 man-year, and continuing costs of 1/4 man-year per year can be expected.

Sampling Plans

A well documented sampling plan for a single media can require 1-2 man months. These resources should be expended at the remote sites.

Quality Control

The recommendations for quality control will require 1 man month of the Q.C. committee, and could require up to 2 man-months for the trained statistician.

CONCLUSIONS AND RECOMMENDATIONS

A list of objectives and sub-objectives to which the data base was designed was prepared. It was determined that the data base was in compliance with all of the objectives so stated. The potential revisions in objectives were presented and discussed. It is recommended that the data manager consider revisions to the input to ultimately allow for system stability while also allowing for system evolution.

A review of the planned equipment purchases by the program manager's office was found to be acceptable. However, Battelle's entry point into the program was too late to have significantly effect in any equipment purchase decisions.

In reviewing the design and structure of the data management activities, the data log books from both field sampling and laboratory analysis were determined to be a very significant component of the overall data management scheme. A formal filing system/library system or management of these records is recommended. Data entries in the Data Management System referencing appropriate log book entries is recommended.

As part of the program study, a list of currently available and accepted models for the transport and restoration of contaminants in the c'emical and biological environments was assembled. It is found from this list that many of the data elements which are stored or planned to be stored in the data base are generally irrelevant to the needs of available computer programs. However, a counter argument to the irrelevancy is that the data base has been designed to take data as collected by the various arsenals, and to store it in a retreival manner. This function is accomplished by the data base admirably. The fault, if any, appears to lie with the data collection exercises, which, in some instances, are conducted without a coal for the use of their data. It is recommended that formal sampling plans be written for all future sampling efforts.*

Finally, the level of inaccuracy associated with standard sampling techniques is much greater than the level of inaccuracy associated with analytical techniques. However, the data base is directed only towards storing the estimate of error associated with the laboratory technique. This process leads to a severe underestimate of the total error associated with each field sample. For this reason the recommendation is that the data item representing laboratory error be dropped, or that some estimate of field error be stored with the data.

A review of quality control procedures is recommended.

The decision on a Management Information System is to be made independent of the Data Management System. It is likely that an MIS would be of overall value on the IR program. Little justification is seen for relating the MIS decision to the data management evaluation.

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* Such requirements are imposed not on excessed sites, but not on active sites with migrating contaminants. The need for sampling plans may be more critical for active sites.